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Flow, Transport, and Reaction during the Conversion of Lignocellulosic Biomass to Fuels and Chemicals: From Hoppers to Bioreactors

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ABSTRACT It is commonly recognized that renewable energy must play an important part in addressing the global challenges of energy security and environmental degradation. While stationary energy needs (residential and industrial) may be largely met by renewable electricity (hydro, solar, wind, etc.), transportation requires the use of energy sources that are mobile and energy dense. Battery and fuel-cell technology are improving, but liquid transportation fuels will remain the primary energy source for transportation, at least for the next few decades. Biochemical conversion of lignocellulosic biomass is one approach to obtaining renewable liquid transportation fuels. The development of computational models for the feedstock handling, enzymatic hydrolysis, and bioreaction unit operations of biochemical conversion will be presented. (1) Unlike simple liquids and gases, the bulk flow and transport of granular materials remain poorly understood by physicists and pose many problems for engineers. While discrete-particle models are considered state-of-the-art for reproducing the mechanics of granular media, continuum models are needed for simulating flows in large vessels, like silos and hoppers. The nonlocal granular fluidity model was implemented in CFD software and demonstrated for a few simple flow geometries. (2) Enzymatic hydrolysis of pretreated biomass involves coupled reaction and mixing of a heterogeneous, multiphase slurry. A coupled CFD and chemical-kinetics model was developed for this reaction, where a sub-cycling strategy was used to circumvent large disparities in time scales with respect to transport physics and chemical kinetics. A novel enzymatic reaction model was used to account for different populations of cellulose with apparent fast- and slow-digestion rates. (3) After sugars are liberated from biomass, they may be biochemically converted to useful fuels or fuel-precursors. Aerobic microorganisms are being considered because of their ability to produce molecules suitable for upgrading and/or blending with hydrocarbon fuels. We developed coupled hydrodynamic, oxygen-transfer, and oxygen-uptake models in CFD software in order to evaluate technical challenges associated with large-scale bioreactor design.

BIO **Dr. Jonathan Stickel** is a Senior Research Engineer in the Biosciences Center of the National Renewable Energy Laboratory. He is performing fundamental and applied research of the fluid mechanics, mass transfer, and reaction kinetics of biomass undergoing conversion to fuels in order to improve overall conversion yields and process economics. Jonathan's graduate research was a theoretical and computational study of concentrated suspension rheology. He was previously employed at Biogen and at Bayer Healthcare, where he worked in downstream process development. He has broad research interests in fluid mechanics, rheology, separation science, reaction engineering, mathematical modeling, and scientific computing. Additional information and a list of publications may be found at https://www.nrel. gov/research/jonathan-stickel.html.

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